potential, and $u(r)$ is the potential at the separation r. The isotherms are shown in Figs. 1(a) and 1(b). In order to obtain a convenient scale, the values of E'/RT and $PV/RT - 1$ for the regular (face-centered cubic) lattice configuration have been subtracted off. For this form of the pair potential, these are given by[9]

$$E'/RT$$

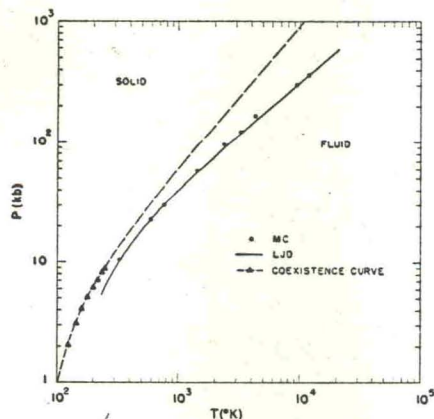$$= 6[1.0110(r/r^*)^{-12} - 2.4090(r/r^*)^{-6}] \quad (2.3)$$

$$PV/RT - 1$$

$$= 24[1.0110(r/r^*)^{-12} - 1.2045(r/r^*)^{-6}].$$

The calculation of points on the Hugoniot curve from these results was done by interpolation in temperature at constant volume and vice versa. In the constant-volume method, the Hugoniot function, the left-hand side of Eq. (2.1a), was
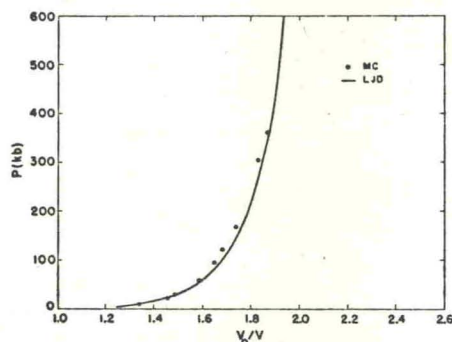
(a)

(b)

Fig. 2. Shock Hugoniots for liquid argon calculated with Monte Carlo (MC) and LJD equations of state using the same pair potential [Eqs. (2.2) and (2.4)]. The pressure colume plane is shown in (a), and the pressure-temperature plane in (b). Also shown in (b) are some experimental points on the fluid-solid coexistence curve and its extrapolation by means of the empirical Simon relation.

[9] J. E. Jones and A. E. Ingham, Proc. Roy. Soc. (London) A107, 636 (1925).

TABLE I. Shock Hugoniots calculated from the Monte Carlo equation-of-state [with Lennard-Jones potential, Eq. (2.4)].

$P(kb)$	V/V_0	$T(°K)$
362	0.535	11 900
305	0.547	9 360
168	0.572	4 330
123	0.595	3 120
96	0.606	2 390
59	0.631	1 401
30	0.673	760
23	0.687	569

calculated for each reduced temperature at the given volume. Three-point interpolation was then used to find the temperature at which Eq. (2.1a) was satisfied, and the remaining equation-of-state quantities were also obtained by interpolation.

Interpolation in volume at constant temperature was complicated by the shape of the isotherms. The probable first-order phase transition, discussed in reference 3 for the isotherm with $kT/\epsilon^* = 2.74$, appears to be present on the higher isotherms also. Because of the small number of points on these isotherms, the dashed curves shown in Figs. 1(a) and 1(b) were sketched in, using only a discontinuity in slope to represent the probable transition. A Hugoniot point on each isotherm was then obtained by interpolation at constant temperature. (On the lowest isotherm, the Monte Carlo points were used directly with three-point interpolation.) As a check on these methods, a Hugoniot point was calculated by the first method from the LJD isotherms of Fig. 1 and found to be in good agreement with an explicit calculation.

In order to transform from reduced thermodynamic variables to real ones, a set of pair potential parameters close to those obtained from second-virial coefficient data were used[10]:

$$\epsilon^*/k = 119.3 \ °K, \qquad r^* = 3.833 \ A, \qquad (2.4)$$

where k is Boltzmann's constant.

The resulting Hugoniot curve is given in Table I and in Figs. 2(a) and 2(b). Also shown in Fig. 2(b) is the extrapolation of the experimental solid-liquid coexistence curve by means of the empirical Simon relation.[11] From this graph it appears that the Hugoniot lies entirely in the fluid region. To shed further light on this point, the loci of Hugoniot points were added to Figs. 1(a) and 1(b). Although the position of the probable transition is poorly

[10] E. Whalley and W. G. Schneider, J. Chem. Phys. 23, 1644 (1955).
[11] D. W. Robinson, Proc. Roy. Soc. (London) A225, 393 (1954).